WEST Search History

Hide Items | Restore | Clear | Cancel

DATE: Monday, March 14, 2005

Hide?	Set Name	Query	Hit Count
		DB=PGPB,USPT; PLUR=YES; OP=ADJ	
☐	L14	L13 and l7	37
☐	L13	20000117	76
☐	L12	L11 and (transform$7 or recombin$7 or genetic or mutat$7)	373
☐	L11	L10 and (mak$7 or synthe$7 or ferment$7 or produ$7 or biosynthe$7)	400
☐	L10	L9 and (fungus or yeast)	400
☐	L9	L8 and amide	872
☐	L8	nitrile hydratase or Nitrilase	1708
☐	L7	L6 or L5 or L4 or L3 or L2 or L1	19409
☐	L6	(564/123)!.ccls.	478
☐	L5	(536/23.2)!.ccls.	12462
☐	L4	(435/254.11)!.ccls.	1447
☐	L3	(435/252.3)!.ccls.	9027
☐	L2	(435/232)!.ccls.	468
☐	L1	(435/129)!.ccls.	167

END OF SEARCH HISTORY

```
=> d his

     (FILE 'HOME' ENTERED AT 13:27:20 ON 14 MAR 2005)

     FILE 'REGISTRY' ENTERED AT 13:27:47 ON 14 MAR 2005
L1             1 S NITRILE HYDRATASE/CN

     FILE 'HCAPLUS' ENTERED AT 13:29:07 ON 14 MAR 2005

     FILE 'REGISTRY' ENTERED AT 13:29:15 ON 14 MAR 2005
                SET SMARTSELECT ON
L2           SEL L1 1- CHEM :        7 TERMS
                SET SMARTSELECT OFF

     FILE 'HCAPLUS' ENTERED AT 13:29:15 ON 14 MAR 2005
L3          1068 S L2
L4            53 S L3 (L) (YEAST OR FUNGUS OR FUNGI)
L5             0 S L4 (L) PREP/RL
L6            18 S L4 (L) AMIDE
L7            16 S L6 AND PD<20000117
L8             8 S L3 (L) CANDIDA
L9             6 S L8 AND PD<20000117
```

=> d

L1 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2005 ACS on STN
RN 82391-37-5 REGISTRY
CN Hydratase, nitrile (9CI) (CA INDEX NAME)
OTHER NAMES:
CN 3-Cyanopyridine hydratase
CN Acrylonitrile hydratase
CN Aliphatic nitrile hydratase
CN E.C. 4.2.1.84
CN Nitrilase
CN **Nitrile hydratase**
MF Unspecified
CI MAN
LC STN Files: AGRICOLA, ANABSTR, BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CAPLUS, CASREACT, CEN, CHEMINFORMRX, CIN, EMBASE, PROMT, TOXCENTER, USPAT2, USPATFULL
DT.CA CAplus document type: Conference; Dissertation; Journal; Patent
RL.P Roles from patents: ANST (Analytical study); BIOL (Biological study); MSC (Miscellaneous); OCCU (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses)
RLD.P Roles for non-specific derivatives from patents: USES (Uses)
RL.NP Roles from non-patents: ANST (Analytical study); BIOL (Biological study); FORM (Formation, nonpreparative); MSC (Miscellaneous); OCCU (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses)
RLD.NP Roles for non-specific derivatives from non-patents: BIOL (Biological study); PROC (Process); PRP (Properties)

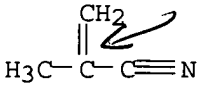
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
503 REFERENCES IN FILE CA (1907 TO DATE)
5 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
504 REFERENCES IN FILE CAPLUS (1907 TO DATE)

```
=> s Methacrylonitrile/cn
L1            1 METHACRYLONITRILE/CN

=> d

L1   ANSWER 1 OF 1  REGISTRY  COPYRIGHT 2005 ACS on STN
RN   126-98-7  REGISTRY
CN   2-Propenenitrile, 2-methyl- (9CI)  (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN   Methacrylonitrile (8CI)
OTHER NAMES:
CN   α-Methacrylonitrile
CN   α-Methylacrylonitrile
CN   1-Methylethenyl cyanide
CN   2-Cyano-1-propene
CN   2-Cyanopropene
CN   2-Methyl-2-propenenitrile
CN   2-Methylacrylonitrile
CN   2-Methylpropenenitrile
CN   Isobutenenitrile
CN   Isopropene cyanide
CN   Isopropenylnitrile
CN   Methacrylnitrile
CN   Methylacrylonitrile
CN   NSC 24145
FS   3D CONCORD
MF   C4 H5 N
CI   COM
LC   STN Files:   AGRICOLA, ANABSTR, BEILSTEIN*, BIOBUSINESS, BIOSIS,
       BIOTECHNO, CA, CANCERLIT, CAOLD, CAPLUS, CASREACT, CBNB, CHEMCATS,
       CHEMINFORMRX, CHEMLIST, CHEMSAFE, CIN, CSCHEM, CSNB, DETHERM*, DIPPR*,
       EMBASE, ENCOMPLIT, ENCOMPLIT2, ENCOMPPAT, ENCOMPPAT2, GMELIN*, HODOC*,
       HSDB*, IFICDB, IFIPAT, IFIUDB, MEDLINE, MRCK*, MSDS-OHS, NIOSHTIC,
       PDLCOM*, PIRA, PROMT, RTECS*, SPECINFO, TOXCENTER, TULSA, USPAT2,
       USPATFULL, VTB
         (*File contains numerically searchable property data)
     Other Sources:   EINECS**, NDSL**, TSCA**
         (**Enter CHEMLIST File for up-to-date regulatory information)
DT.CA  CAplus document type:  Conference; Dissertation; Journal; Patent;
       Preprint; Report
RL.P   Roles from patents:  ANST (Analytical study); BIOL (Biological study);
       FORM (Formation, nonpreparative); MSC (Miscellaneous); OCCU
       (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); RACT
       (Reactant or reagent); USES (Uses); NORL (No role in record)
RLD.P  Roles for non-specific derivatives from patents:  ANST (Analytical
       study); BIOL (Biological study); PREP (Preparation); PROC (Process); PRP
       (Properties); RACT (Reactant or reagent); USES (Uses)
RL.NP  Roles from non-patents:  ANST (Analytical study); BIOL (Biological
       study); FORM (Formation, nonpreparative); MSC (Miscellaneous); OCCU
       (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); RACT
       (Reactant or reagent); USES (Uses); NORL (No role in record)
RLD.NP Roles for non-specific derivatives from non-patents:  BIOL (Biological
       study); FORM (Formation, nonpreparative); PREP (Preparation); PROC
       (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses)
```

unsat, See Rezende et al UFMG-45.



NiceZyme View of ENZYME: EC 4.2.1.84

Official Name
Nitrile hydratase.
Alternative Name(s)
Nitrilase.
Reaction catalysed
An aliphatic amide <=> a nitrile + H(2)O
Comments
• Acts on short-chain aliphatic nitriles, converting them into the corresponding acid amides. • Does not act on these amides or on aromatic nitriles (cf. EC 3.5.5.1).

Cross-references	
BRENDA	4.2.1.84
EMP/PUMA	4.2.1.84
PRIAM enzyme-specific profiles	4.2.1.84
WIT	4.2.1.84
Kyoto University LIGAND chemical database	4.2.1.84
IUBMB Enzyme Nomenclature	4.2.1.84
IntEnz	4.2.1.84
MEDLINE	Find literature relating to 4.2.1.84
Swiss-Prot	P21219, NHA1_RHORH ; P29378, NHA2_RHORH ; P27764, NHAA_PSECL ; P97051, NHAA_PSEPU ; Q7SID2, NHAA_PSETH ; P13448, NHAA_RHOER ; Q53118, NHAA_RHOSO ; P27763, NHAB_PSECL ; P97052, NHAB_PSEPU ; Q7SID3, NHAB_PSETH ; P13449, NHAB_RHOER ; Q53117, NHAB_RHOSO ; P21220, NHB1_RHORH ; P29379, NHB2_RHORH ;

View entry in original ENZYME format

All Swiss-Prot entries referenced in this entry, with possibility to download in different formats, align etc.

All ENZYME/Swiss-Prot entries corresponding to 4.2.1.- new
All ENZYME/Swiss-Prot entries corresponding to 4.2.-
All ENZYME/Swiss-Prot entries corresponding to 4.-

Root

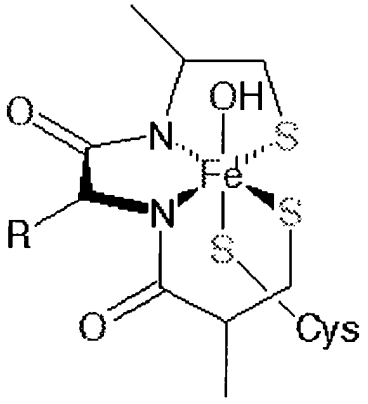
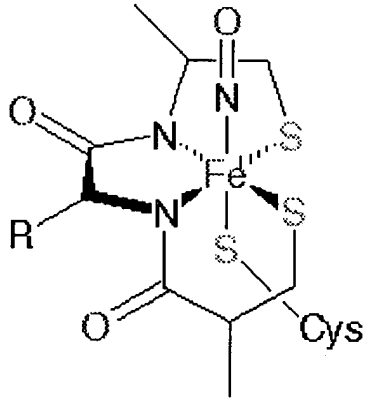
PROMISE mirror: http://metallo.scripps.edu/PROMISE/
hosted at TSRI's MDB (USA): http://metallo.scripps.edu/

Mononuclear iron proteins

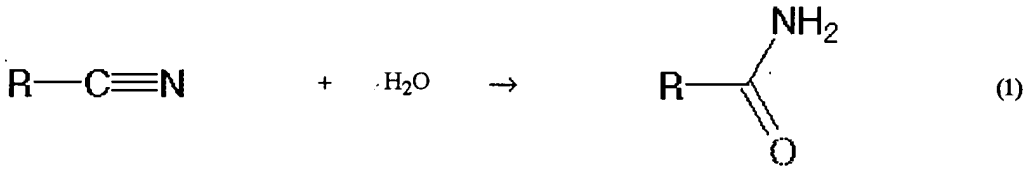
Nitrile hydratase

Created: 29 January 1998
Last modified: 11 November 1998

Nitrile hydratase

Mononuclear iron centre		Iron ligands	Formal iron oxidation/spin states
Activated	Resting		
		$3 \times S^{\gamma}_{Cys}$; $2 \times N^{\alpha}$; OH^- or ·NO	Fe^{III} (S=1/2)
$(S^{\gamma}_{Cys})_3(N^{\alpha})_2OH$	$(S^{\gamma}_{Cys})_3(N^{\alpha})_2NO$		

Nitrile hydratase and amidase are the two hydrolytic enzymes responsible for the sequential metabolism of nitrile compounds in some bacteria and fungi which are capable of utilising aliphatic nitriles as the sole source of nitrogen and carbon [1-3]. Nitrile hydratases (NHases; EC 4.2.1.84) are mononuclear iron or (noncorrinoid) cobalt enzymes that catalyse the hydration of a large number of diverse nitriles to their corresponding amides:



(1)

Organisms expressing NHases are capable of utilising aliphatic nitriles as the sole source of nitrogen. NHases have been efficiently used for the industrial production of acrylamide from acrylonitrile [1] and for removal of nitriles from wastewater [4]. Photosensitive NHases intrinsically possess nitric oxide (·NO) bound to the iron centre and its photodissociation activates the enzyme. These enzymes are composed of two types of subunits, α and ß, which are not related in amino acid sequence. NHases exist as αß dimers or $\alpha_2\beta_2$ tetramers and bind one iron ion per αß unit.

The 3D structures of photoactivated NHase from *Rhodococcus* sp. R312 [5] and nitrosylated NHase from *Rhodococcus* sp. N771 [6] have been determined. The enzyme exists as an αß dimer. The α subunit consists of a long extended Nterminal 'arm' (residues 10-52), containing two αhelices, and a Cterminal domain with an unusual fourlayered structure (αßßα). The ß subunit consists of a long 30residue Nterminal loop that wraps around the α subunit; a helical domain (residues 30-112) that packs with Nterminal domain of the α subunit; and a Cterminal domain consisting of a ßroll and one short helix.

The metal centre is located in the central cavity at the interface between two subunits. All protein ligands to the iron are provided by the α subunit. The protein ligands to the iron are the sidechains of the three Cys residues and two mainchain amide nitrogens. The lowspin Fe^{III} ion is octahedrally coordinated, with the protein ligands at the five vertices of an octahedron; the sixth position, accessible to the active site cleft, is occupied either by ·NO or by a solvent exchangeable ligand (hydroxide or water) [7]. In *Rhodococcus* sp. N771 NHase, two Cys residues coordinated to the iron were found to be posttranslationally modified to Cys-sulphinic (Cys-SO_2H) and -sulphenic (Cys-SOH) acids. Together with oxygen of the Ser residue, these modifications induced a 'claw' setting of oxygen atoms capturing an NO molecule [6]. A role for the iron centre in catalysis remains unclear. Mechanistic proposals were made which all suggest that the metal ion acts as a Lewis acid [5]. The table below lists the mononuclear iron environment residues in known 3D structures.

Enzyme	Mononuclear iron environment residues (α subunit)				Fe sixth ligand	PDB code	Ref.
Rhodococcus sp. R312	Cys110 (S^{γ})	Cys113 (S^{γ}, N^{α})	Ser114 (N^{α})	Cys115 (S^{γ})	OH^-	1ahj	[5]
Rhodococcus sp. N771	Cys109 (S^{γ})	Cys-SO_2H112 (S^{γ}, N^{α})	Ser113 (N^{α})	Cys-SOH114 (S^{γ})	·NO	-	[6]

■

NHase in enzyme databases

ENZYME	LIGAND	BRENDA	UMBBD	Official name	Alternative names
4.2.1.84	4.2.1.84	4.2.1.84	e0067	Nitrile hydratase	Acrylonitrile hydratase; NHase; nitrilase

■

NHase in alignment databases

Protein Family	Pfam	LPFC 3D alignment
20343; nitrile hydratase α chain	-	-
80462; nitrile hydratase ß chain	-	-

■

NHase in 3D databases

Nitrile hydratase contains a single iron atom.

Display in the MDB Viewer

PDB	scop	BSM	RELI Base	Header	MACROMOLECULAR STRUCTURES
1ahj	-	1ahj	1ahj	Nitrile hydratase; *Rhodococcus* sp. R312	-

[1] Macromolecular Structures abstract. Full text is available to BioMedNet Members

References

1. Yamada, H. and Kobayashi, M. (1996) Nitrile hydratase and its application to industrial production of acrylamide. *Biosci. Biotechnol. Biochem.* **60**, 1391-1400.
2. Nawaz, M.S., Heinze, T.M. and Cerniglia, C.E. (1992) Metabolism of benzonitrile and butyronitrile by *Klebsiella pneumoniae*. *Appl. Environ. Microbiol.* **58**, 27-31.
3. Linardi, V.R., Dias, J.C. and Rosa, C.A. (1996) Utilization of acetonitrile and other aliphatic nitriles by a *Candida famata* strain. *FEMS Microbiol. Lett.* **144**, 67-71.
4. Wyatt, J.M. and Knowles, C.J. (1995) The development of a novel strategy for the microbial treatment of acrylonitrile effluents. *Biodegradation* **6**, 93-107.
5. Huang, W., Jia, J., Cummings, J., Nelson, M.J., Schneider, G. and Lindqvist, Y. (1997) Crystal structure of nitrile hydratase reveals a novel iron centre in a novel fold. *Structure* **5**, 691-699.
6. Nagashima, S., Nakasako, M., Dohmae, N., Tsujimura, M., Takio, K., Odaka, M., Yohda, M., Kamiya, N. and Endo, I. (1998) Novel nonheme iron center of nitrile hydratase with a claw setting of oxygen atoms. *Nature Struct. Biol.* **5**, 347-352.
7. Scarrow, R.C., Brennan, B.A., Cummings, J.G., Jin, H., Duong, D.J., Kindt, J.T. and Nelson, M.J. (1996) Xray spectroscopy of nitrile hydratase at pH 7 and 9. *Biochemistry* **35**, 10078-10088.


Bibliography on structural studies of nitrile hydratase


Reviews on nitrile hydratase